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On the Lamb-shift and the ionisation energy of helium-like atoms

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The ionisation energies of helium-like atoms have been calculated non-relativistically by HYLLERAAS, using a variational method, and relativistically by ERIKSSON.[1] The energies came out higher than the experimental data, contrary to what might have been expected from the method. ERIKSSON[2] has suggested that this discrepancy might be removed by considering the electromagnetic level shift discovered in the spectrum of hydrogen by LAMB and RETHERFORD.[3]

BETHE[4, 5] has given the following expression for the level shift of hydrogen-like atoms in a quantum state a:

$$W(a) = \frac{2\alpha}{3\pi}\left(\frac{1}{mc}\right)^2 \sum_n |\boldsymbol{p}_{an}|^2 (E_n - E_a)\, {}^e\log \frac{mc^2}{|E_n - E_a|} \tag{1}$$

$$= \frac{2\alpha}{3\pi} S(a)\, {}^e\log \frac{mc^2}{\epsilon(a)}, \qquad \alpha = \frac{e^2}{\hbar c}, \tag{2}$$

where

$$S(a) = \left(\frac{1}{mc}\right)^2 \sum_n |\boldsymbol{p}_{an}|^2 (E_n - E_a), \tag{3}$$

thus defining an average excitation energy $\epsilon(a)$.

On certain conditions, these formulae can be used approximately also for atoms with N electrons. Generalizing then the transformation of $S(a)$ used by BETHE, we get

$$S_N(a) = -\left(\frac{\hbar}{mc}\right)^2 \int^{(3N)} \psi_a^* \sum_{i=1}^{N} \sum_{j=1}^{N} \nabla_i V \cdot \nabla_j \psi_a \prod_{k=1}^{N} d\boldsymbol{r}_k, \tag{4}$$

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[1] H. A. S. ERIKSSON, Zs. f. Phys., *109*, 762, 1938.

[2] H. A. S. ERIKSSON, Nature, *161*, 393, 1948.

[3] W. E. LAMB Jr. and R. C. RETHERFORD, Phys. Rev., *72*, 241, 1947.

[4] H. A. BETHE, Phys. Rev., *72*, 339, 1947.

[5] H. A. BETHE, Solvay Report, 1948.

where

$$V = \sum V_\mu + \sum_{\mu<\nu}\sum V_{\mu\nu}, \quad V_\mu = -\frac{Z e^2}{r_\mu}, \quad V_{\mu\nu} = \frac{e^2}{r_{\mu\nu}}, \quad \nabla_\mu^2 V_\mu = 4\pi Z e^2 \delta(\boldsymbol{r}_\mu),$$

or

$$S_N(a) = 2 N \pi Z e^2 \left(\frac{\hbar}{m c}\right)^2 \int^{(3N-3)} [\psi_a^2]_{r_i=0} \prod_{\substack{k=1\\k\neq i}}^{N} d\,\boldsymbol{r}_k. \tag{5}$$

For the ground state of H-like and He-like atoms we get respectively:

$$S_1(1s) \quad = 4 Z^4 \alpha^2 Ry, \qquad 1\,Ry = \frac{m e^4}{2\hbar^2}, \tag{6}$$

and

$$S_2((1s)^2) = 8 P(Z) \alpha^2 Ry, \quad P(Z) = Z(Z-5/16)^3, \tag{7}$$

using in the latter case a screening wave function

$$\psi_a = (Z-5/16)^3/(\pi a_0^3) \exp\left[-(Z-5/16)(r_1+r_2)/a_0\right], \quad a_0 = \hbar^2/(m e^2).$$

The radiative correction of the ionisation energy of He-like atoms in the ground state is expressed by:

$$J((1s)^2) = W_2((1s)^2) - W_1(1s) =$$
$$= \frac{8}{3\pi}\alpha^3 Ry \left[2 P(Z)\, {}^e\!\log \frac{2\alpha^{-2}}{Z^2 \epsilon_2((1s)^2)} - Z^4\, {}^e\!\log \frac{2\alpha^{-2}}{Z^2 \epsilon_1(1s)}\right]. \tag{8}$$

The average excitation energy has been obtained by numerical integration[1], and is found to be $\epsilon_1(1s) = 19{,}76\ Ry$, for the ground state of hydrogen. For He-like atoms the two alternatives have been used, viz.

$$\epsilon_2((1s)^2) = \epsilon_1(1s), \tag{9: I}$$

$$Z^2 \epsilon_2((1s)^2) = (Z-1)^2 \epsilon_1(1s), \tag{9: II}$$

giving respectively

$$J_{\mathrm{I}}((1s)^2) = [2P(Z) - Z^4][3.775 - {}^e\!\log Z] \cdot 0.0724\ \mathrm{cm}^{-1} \tag{10: I}$$

and

$$J_{\mathrm{II}}((1s)^2) =$$
$$= \left\{[2P(Z) - Z^4]\ [3.775 - {}^e\!\log(Z-1)] + Z^4\, {}^e\!\log\frac{Z}{Z-1}\right\} \cdot 0.0724\ \mathrm{cm}^{-1}. \tag{10: II}$$

J_{I} and J_{II} are tabulated below. The third last column gives the discrepancies between the relativistic ionisation energies calculated by ERIKSSON[2] and by ROBINSON[3] and the measurements by TYRÉN[4] and by FLEMBERG[5]. The unit is cm^{-1}.

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[1] The author wishes to thank Dr. P. KUHN for his assistance in the numerical work.

[2] H. A. S. ERIKSSON, Zs. f. Phys., *109*, 762, 1938.

[3] H. A. ROBINSON, Phys. Rev. *51*, 14, 1937.

[4] F. TYRÉN, Nova Acta Reg. Soc. Sci. Upsaliensis, IV, *12*, No. 1, 1940.

[5] H. FLEMBERG, Arkiv f. Mat., Astr., Fys., *28 A*, No. 18, 1942.

Table.

Z	Ionisation energy					Discrepancy calc.-exp.	J_{I}	J_{II}
	nonrelativistically HYLLERAAS modified by ROBINSON[1]	relativity correction ERIKSSON[2]	mass pol. corr. ROBINSON[1]	calculated total	experimental[3, 4]			
2	198322	2	−5	198319	198314 ± 5	+ 5	0.7	1.7
3	610058	38	−4	610092	610079 ± 25	+ 13	6.9	10
4	1241151	161	−3	1241309	1241225 ± 100	+ 84	25	34
5	2091672	484	−1	2092155	2091960 ± 200	+ 195	64	80
6	3161626	1135	0	3162761	3162450 ± 300	+ 311	131	160
7	4451052	2284	+1	4453337	4452800 ± 500	+ 537	237	282
8	5959945	4133	+2	5964080	5963000 ± 600	+1080	390	460
9	7688318	6923	+3	7695244	7693400 ± 800	+1844	599	700
12	14190202	23853	+6	14214061	14209200 ± 2500	+4861	1642	1880
13	16796463	33497	+6	16829966	16825000 ± 3000	+4966	2150	2460

[1] H. A. ROBINSON, Phys. Rev., *51*, 14, 1937.

[2] H. A. S. ERIKSSON, Zs. f. Phys., *109*, 762, 1938.

[3] F. TYRÉN, Nova Acta Reg. Soc. Sci. Upsaliensis, IV, *12*, No. 1, 1940.

[4] H. FLEMBERG, Arkiv f. Mat., Astr., Fys., *28 A*, No. 18, 1942.

When calculated from Bethe's nonrelativistic approximation, the radiative correction accounts for about one half of the discrepancy between the earlier theory and experiment. As can be seen from the expressions (10), this approximation is, however, doubtful for higher values of Z.

Furthermore, in arriving at the expression (1), Bethe neglects a term $(E_n - E_a)$ in comparison with mc^2 in the numerator of the logaritmic factor, thus imposing the condition $Z \ll 40$, if we assume $\epsilon \sim 20\ Ry$. The retention of this term is, however, quantitatively insignificant in those cases considered here and has to be examined in connection with other approximations. To settle this inconsistency a relativistic calculation of the radiative correction has been undertaken.

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